Asymmetric PML for the Absorption of Waves. Application to Mesh Refinement in Electromagnetic Particle-In-Cell Plasma Simulations.[1]

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1 Introduction

We present an extension of the original Bérenger formulation of the Perfectly Matched Layer [1] with additional terms and tunable coefficients. Under certain constraints on the coefficients, the newly introduced "medium" does not generate any reflection at any angle or any frequency and is thus a Perfectly Matched Layer (PML). Unlike the original PML, however, the new formulation introduces some asymmetry in the absorption rate and is therefore labeled APML for Asymmetric Perfectly Matched Layer.

Taking advantage of the high rates of absorption of the APML, we have devised a new strategy for introducing the technique of Mesh Refinement into electromagnetic Particle-In-Cell plasma simulations. Previous attempts have relied on algorithms of various complexity to connect calculations of EM fields at the border of regular grids at different resolutions (we will refer these as "sewing" algorithms). Most were unstable at small wavelengths while the stable ones suffered form inherent limitations on their ability to avoid spurious wave reflection at interfaces and were complicated to implement [5]. Instead, we propose a technique by substitution. We will present the details of the algorithm as well as 2-D examples of its application to laser-plasma interaction in. the context of fast ignition.

2 Definition of the APML

For the transverse electric (TE) case, we define the APML as

$$\varepsilon_0 \frac{\partial E_x}{\partial t} + \sigma_y E_x = \frac{c_y}{c}\frac{\partial H_z}{\partial y} + \overline{\sigma}_y H_z \quad (1)$$

$$\varepsilon_0 \frac{\partial E_y}{\partial t} + \sigma_x E_y = -\frac{c_x}{c}\frac{\partial H_z}{\partial x} + \overline{\sigma}_x H_z \quad (2)$$

$$\mu_0 \frac{\partial H_{zx}}{\partial t} + \sigma^*_x H_{zx} = -\frac{c^*_x}{c}\frac{\partial E_y}{\partial x} + \overline{\sigma}^*_x E_y \quad (3)$$

$$\mu_0 \frac{\partial H_{zy}}{\partial t} + \sigma^*_y H_{zy} = \frac{c^*_y}{c}\frac{\partial E_x}{\partial y} + \overline{\sigma}^*_y E_x \quad (4)$$

$$H_z = H_{zx} + H_{zy} \quad (5)$$

For $c_x = c_y = c^*_x = c^*_y = c$ and $\overline{\sigma}_x = \overline{\sigma}_y = \overline{\sigma}^*_x = \overline{\sigma}^*_y = 0$, this system reduces to the Berenger PML medium, while adding the additional constraint $\sigma_x = \sigma_y = \sigma^*_x = \sigma^*_y = 0$ leads to the system of Maxwell equations in vacuum.

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It can be shown [4] that if $c_x = c_x^*$, $c_y = c_y^*$, $\overline{\sigma}_x = \overline{\sigma}_x^*$, $\overline{\sigma}_y = \overline{\sigma}_y^*$, $\frac{\sigma_x}{\varepsilon_0} = \frac{\sigma_x^*}{\mu_0}$ and $\frac{\sigma_y}{\varepsilon_0} = \frac{\sigma_y^*}{\mu_0}$ then the impedance of an APML medium is $Z = \pm\sqrt{\mu_0/\varepsilon_0}$, which is the impedance of vacuum. Hence, like the PML, given some restrictions on the parameters, the APML does not generate any reflection at any angle and any frequency. Just as for the PML, this property is not retained after discretization [4].

We assume that we have an APML layer of thickness δ (measured along x) and that $\sigma_y = \overline{\sigma}_y = 0$ and $c_y = c$. The coefficient of reflection given by this layer is

$$R_{APML}(\theta) \quad = \quad e^{-2(\sigma_x \cos\varphi/\varepsilon_0 c_x)\delta} \tag{6}$$

which happens to be the same as the PML theoretical coefficient of reflection if we assume $c_x = c$. Hence, it follows that for the purpose of wave absorption, the term $\overline{\sigma}_x$ seems to be of no interest. However, although this conclusion is true at the infinitesimal limit, it does not hold for the discretized counterpart.

We will present the numerical considerations that have led us to introduce such a medium as well as its theory. Several finite-difference numerical implementations are derived and the performance of the APML is contrasted with that of the PML in one and two dimensions. Using plane wave analysis, we show that our APML implementations lead to higher absorption rates than the considered PML implementations (Fig.1).

3 Mesh refinement by substitution

We propose a technique by substitution using the following procedure:

1. a usual EM-PIC calculation is performed on a grid G at resolution R1,
2. in an area A where one is interested in a higher resolution R2, we perform electromagnetic PIC calculations on
   (a) a patch P1 at resolution R1,
   (b) a patch P2 at resolution R2,

   both covering A and being terminated by an APML,
3. the EM force F acting on a macroparticle is F(G) outside A and is F(G)-F(P1)+F(P2) inside, where F(α) means the force resulting from the fields computed on grid (or patch) α.

The immediate advantage of the procedure over a more standard grid "sewing" technique is its simplicity since no special (and often cumbersome) algorithm is needed at grid interfaces. Also, since it allows the use of very efficient absorbing boundary conditions, it offers very high order wave absorption at any angle at the interface, while other algorithms are usually limited to first or second order absorption algorithms with respect to wavelength and angle.

One possible drawback of this technique is the fact that inside a refined area, the field calculation is performed three times: one in the fine resolution patch, one in the coarse resolution patch and one on the main grid in the refined area. However, for a refinement factor of two, the

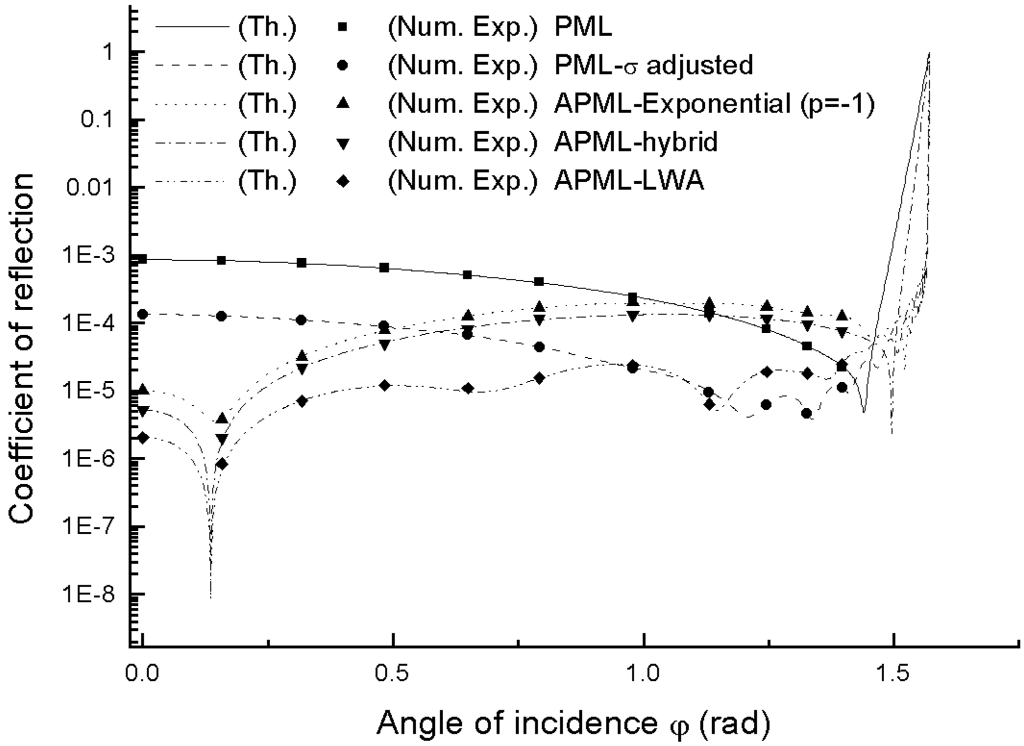

Figure 1: Coefficient of reflection of various PML and APML implementations as a function of angle of incidence for a plane wave excited with a period $\tau = 2\pi/\omega = 20\delta x/c$ where δx is the mesh size. Theoretical (Th.) and numerical experiment (Num. Exp.) results are displayed.

additional cost (compared to a sewing method) is 50% in 2-D and 25% in 3-D, which we consider minor given the advantages in accuracy and simplicity offered by the new technique. An additional amount of work also comes from the use of absorbing layers but here again, we believe that the benefits largely outweight the inconvenience.

Another source of additional work comes from the charge deposition and force gathering onto and from the grids which has to be done on the three grids in the refined area. However, if the gather and scatter use linear weightings (the standard in PIC calculations), the charge depostion needs to be done on the fine grid only and then propagated to the coarse patch and main grid; likewise, the field can be summed from every grid to an auxilliary grid of resolution R2 and then gathered onto particles. In this way, there is no penalty on the expensive gather/scatter part and only minimal additional work.

A question which arises with this method concerns the treatment of the macroparticles entering and exiting the patches P1 and P2. Ideally, the macropaticles should enter (exit) a patch and their corresponding field should magically appear (vanish) as if the particle was coming from (departing to) infinity. These conditions may be challenging to achieve and we have opted for an operationally simple procedure: the current of a macroparticle M of charge q is deposited inside a patch as soon as it enters it and stops being deposited as soon as it leaves the refined area. The consequence is the creation of a macroparticle of charge -q at the entrance point after the entrance of M and a macroparticle of charge q standing at the exit point after the exit of M.

Although these are spurious charges that should not be present ideally, their effect should be minimal inside the patch because of the cancellation F(P2)-F(P1). Nevertheless, a residual spurious force is present due to this effect and it may be necessary to reduce it or, if possible, suppress it if it proves to be a problem. One method of suppressing the spurious force consists of depositing the current inside the APML patch in a manner that prevents the appearance of these spurious charges. Another way would be to periodically apply a correction on the static part of the field using a "Boris", "Marder-Langdon", or hyperbolic correction [2, 3, 6].

4 Examples

We have implemented the new mesh refinement scheme in the 2-D electromagnetic Particle-In-Cell Emi2d developed at Ecole Polytechnique. We will present 2-D examples and tests of application to laser-plasma interaction in the context of fast ignition, using a homogeneous cylindrical target as well as a rectangular target with a ramp in density.

5 Conclusion

We have presented a new asymmetric PML (labeled APML) which is formally an extension of Bérenger's original formulation and have demonstrated that the discretized APML offers superior absorption rates than discretized PML under a plane wave analysis. Building upon this, we have devised a new strategy for implementing mesh refinement in electromagnetic Particle-In-Cell codes, relying on field substitution between patches terminated by an APML layer. Results obtained from application to laser-plasma interaction in the context of fast ignition are promising. Although we have considered the finite-difference discretization of Maxwell-like equations only, the APML system of equations, as well as the new mesh refinement scheme, may be used with other discretization schemes, such as finite element, and may be applied to other wave equations for applications beyond electromagnetics.

References

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